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<p>To limit the responses of constraint spectra to the noise level of the instrument and maximize the response of a target spectrum, computer optimization programs are usually used. Computer capacity however limits the number of constraints that can be considered at one time. A need exists to select a representative set of independent constraint spectra which will be adequate for all situations. Through the use of factor analysis such a representative set was chosen. It is believed to come close to meeting the necessary requirements.</p>		

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PREFACE

The work reported was carried out May 1976 through April 1977 under Task 1W762710AD2702, Remote Sensing Alarm Techniques. The latter task constitutes authorization for the work.

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CONTENTS

	<u>Page</u>
I. INTRODUCTION	7
II. SPECTRAL DATA FILE	8
A. Backgrounds	8
B. Interferences	14
III. CLASSIFICATION METHODS	14
A. Inspection	16
B. Correlation Analysis	18
1. Theory	18
2. Results	19
C. Linear-Programming Method	22
D. Factor Analysis	24
1. Theory	24
2. Results	28
IV. CONCLUSIONS	32
LITERATURE CITED	33
APPENDIXES	
A. Derivation of F_{Rj} Equation	35
B. Ten Factor Constraints	37
C. Thirty-seven Spectra Chosen as Constraints from the Factor Analysis Technique	41
DISTRIBUTION LIST	47

CONTENTS (Contd)

LIST OF FIGURES

<u>Figure</u>		<u>Page</u>
1	Twelve-Hour Background Run	10
2	Slope Variations with Equal Ozone Intensity	10
3	Spectral Changes Due to Varying Cloud Cover	11
4	LAS with Positive Ozone Peak	11
5	Two Spectra of Unknown Origin and Their LAS Background	12
6	Negative Response from Spectra of Unknown Origin	12
7	Four Terrain Spectra	13
8	Spectral Variations of a Snow-Capped Mountain Range	13
9	Explosion Sequence	14
10	Four Dust Spectra	14
11	Three Interference Spectra	16
12	Similar Spectra	17
13	LAS with High Ozone Intensity	18
14	LAS Spectra with Correlation Value of 1.0000	21
15	LAS Spectra with Correlation Value of 0.8991	21
16	First 10 Rotated Loadings from LAS Data File	29

LIST OF TABLES

<u>Table</u>		
1	Eigenvalues and Eigenvalue Ratios for the First 20 Factors from the LAS Data File	29
2	Factor Scores for LAS Spectra Meeting the Boundary Conditions	30

SPECTRAL CLASSIFICATION TECHNIQUES FOR REMOTE-SENSING ALARMS

I. INTRODUCTION.

The remote sensing of toxic chemical agent clouds requires discrimination techniques that minimize responses due to background changes and interferences while maintaining adequate agent response. Because of the large number of possible variations in agents, backgrounds and interferences, most techniques use computer optimization programs to find a discrimination function. Such programs are usually designed to maximize the response of some target spectrum (the agent), while limiting the responses of all the constraint spectra (backgrounds and interferences) to the noise level of the instrument. Since computer capacity restricts the number of constraints that can be used at any one time, there exists a need for a classification system to select a representative set of independent background and interference spectra that serve as adequate constraints in all situations. In addition, the system should be capable of examining newly obtained spectra and rejecting those found to be similar to existing constraints. The purpose of this report is to describe the classification methods tried to date and to construct a file of independent spectra using the most appropriate technique.

The data used to examine the classification methods were difference energy spectra from the exploratory development (XD) Passive LOPAIR. It is composed of two subsystems: a spectroradiometer and a discriminator.

The spectroradiometer uses a circular variable filter (CVF) and a nitrogen cooled Hg:Cd:Te detector. The CVF covers half of a wheel that rotates at 1 Hz. A chopper, which is mechanically connected to the rotating filter wheel, rotates at 1000 Hz with the detector alternately viewing the scene and an internal blackbody. This chopping produces an ac signal whose peak-to-peak amplitude is proportional to the energy difference between the background and the internal blackbody. The ac signal is normalized by automatic gain control and demodulated to produce a continuous difference energy spectrum of the 8.4 to 12.5 μm region. The AGC maintains a constant amplitude of ± 3.0 volts depending on whether the scene is hotter or cooler than the internal blackbody. The field stop of the CVF is set so that the spectroradiometer has about 1% spectral bandwidth, but the actual spectral resolution is about 2%.

The discriminator is a small, special-purpose, hybrid computer, which computes the absolute value of

$$\int_{\lambda_1}^{\lambda_2} c(\lambda)x(\lambda)d\lambda$$

where

$C(\lambda)$ is the coefficient value

$X(\lambda)$ is the signal value

λ_1 is the beginning of the first channel

λ_2 is the end of the last channel.

The discriminator can accept up to sixteen channels, where a channel is defined as any part of the difference energy spectrum with bandwidth ranging from zero to the full spectral range of the instrument. To account for minor variations in instrument responsivities, this range was limited to 8.68 to 11.83 μm .

The signal from each channel is weighted by an op-amp whose effective gain is proportional to the channel coefficient. The weighted outputs of all channels are summed by an integrating network with a time constant of 0.1 sec. The integrator is discharged with a time constant of 2.7 sec, thus averaging the present value with previous values to improve the signal-to-noise ratio of the discriminator output.

This output is the instrument's response which can be either a positive or negative voltage. Typically, the discriminant functions were designed to produce a positive response for a target.

The LOPAIR spectra were standardized by dividing by the instrument's responsivity curve, and normalized by dividing by the maximum absolute value. Both field spectra and simulated field spectra from laboratory measurements were included in the data file. The spectra were initially categorized according to their physical type: that is low-angle sky, terrain, dust, etc.

II. SPECTRAL DATA FILE.

The data file consists of agents, simulants, interferences and backgrounds. The classification techniques are applied only to the spectra being used as constraints: that is, interferences and backgrounds. The set of backgrounds includes low-angle sky (LAS), terrain, and combinations of both. Interferences include dusts, smokes, decontaminants and explosions.

A. Backgrounds.

The background data set consists of 86 LAS and 9 terrain (or combination) spectra.

The significant features in any LAS spectrum are the intensity of the ozone peak and the slope of the spectrum. For the purpose of this study, the ozone intensity is defined as the magnitude of the spectrum at 9.65 μm , the approximate center of the doublet. Ozone

intensity and slope vary with changes in ambient temperature, cloud cover, ozone concentration, atmospheric transmittance, and angle of observation. Given a fixed angle of instrument elevation, cloud cover variations are responsible for most spectral changes in a continuous 12-hour period. Changes resulting from variations in ambient temperature and atmospheric transmittance are usually gradual and of a lower magnitude. Most variations in ozone concentration occur over a long time period and have a small effect in relation to the other parameters. At small angles (0° to 10°), changes in instrument elevation can produce significant variations in the spectrum.² These variations are presumed to be equivalent to combinations of changes in the other parameters.

Figure 1 contains 11 LAS spectra showing variations primarily in ozone intensity. These spectra came from a 12-hour background test that began in partly cloudy skies (last spectrum) and ended in a snowstorm (first four spectra). The instrument had a fixed angle throughout the test, and the ambient temperature varied only 5°C over the entire run. The spectral changes are due primarily to cloud cover variations, with decreasing atmospheric transmittance occurring as the snow increased.

Figure 2 shows five spectra having nearly the same ozone intensity, but different slopes. The spectra were obtained on clear days in the fall, winter, and spring, and reflect changes in all parameters except cloud cover.

Figure 3 shows five spectra in which both slope and ozone intensity vary. These spectra were taken over a 5-minute time period with changes due entirely to varying cloud cover.

Occasionally, situations occur where the LAS spectrum contains a peculiar feature of uncertain origin. Figure 4 shows one example from a field test at Yuma, Arizona. Note that the ozone peak crosses the zero point. This implies that the upper layers of the atmosphere which contain ozone are at a higher temperature than the surface layer, an unusual occurrence for those altitudes. The exact cause is unknown.

Figure 5 shows three spectra obtained from a background run at Aberdeen Proving Ground. The first spectrum was typical of the run. The remaining two spectra were taken from a variation that lasted about 5 minutes and caused a considerable negative response (figure 6). The shape and duration of the response plot indicates that the probable cause was a solar transit near the field of view of the instrument.

Abnormal occurrences such as those usually cause a response, but are difficult to classify because their features are unique. They are generally added to the constraint file, but they probably would not prevent responses to spectra that are similar, but not identical. Spectra such as these are not classified because of their uncertain origins.

The terrain data file consists of just nine spectra. The spectra of trees, water and soil appear similar to blackbodies, but contain reflected ozone components (figure 7). Mountains, and other features with varying surface compositions can have unusual and unpredictable spectra, particularly under direct sunlighting. Figure 8 shows three spectra of similar looking areas on a snowcapped mountain range under nearly the same lighting conditions. The reflected ozone

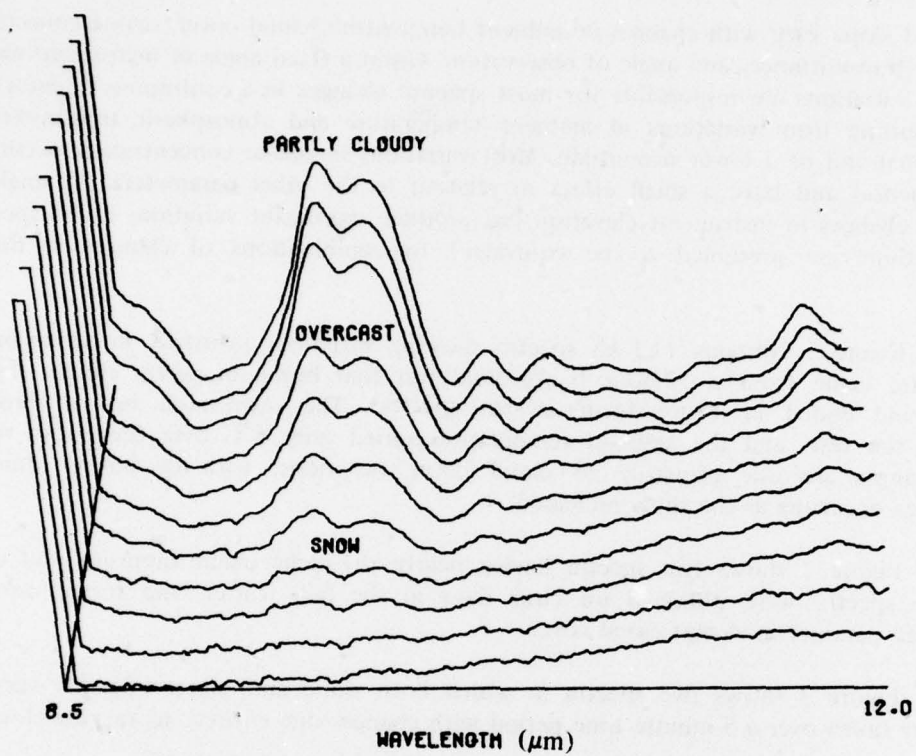


Figure 1. Twelve-Hour Background Run

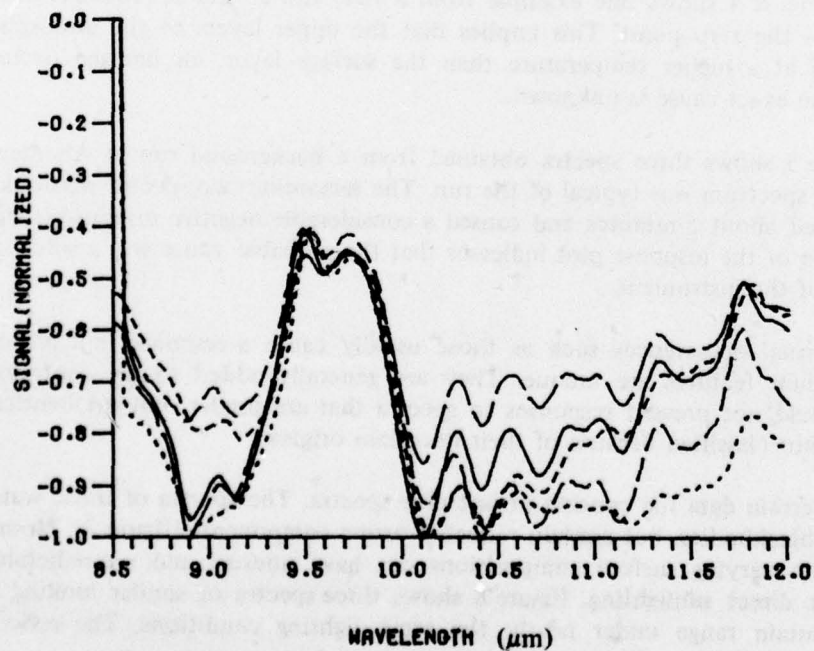


Figure 2. Slope Variations with Equal Ozone Intensity

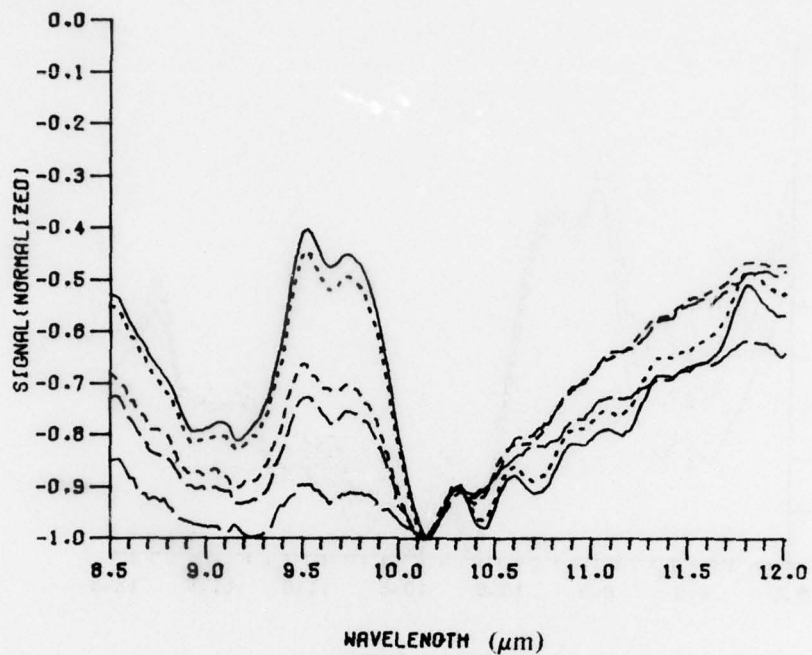


Figure 3. Spectral Changes Due to Varying Cloud Cover

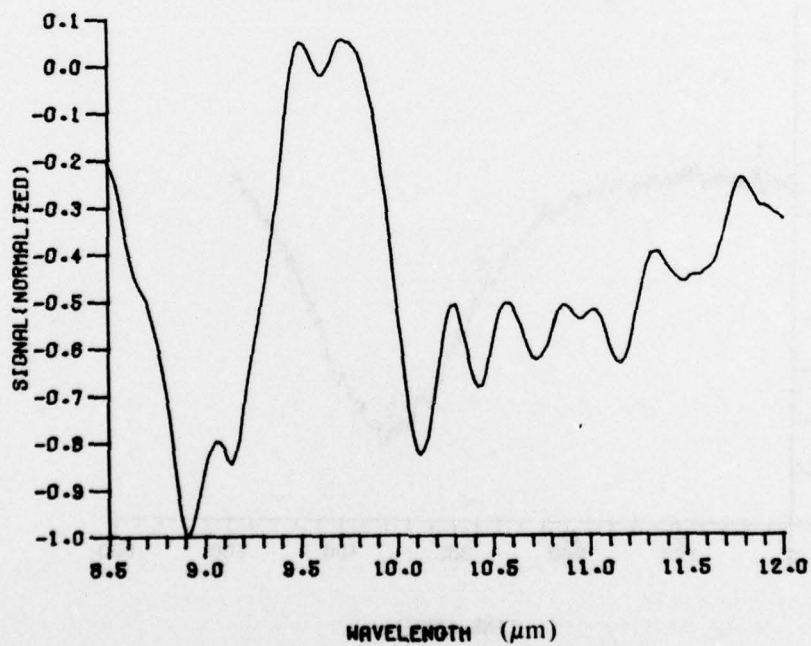


Figure 4. LAS with Positive Ozone Peak

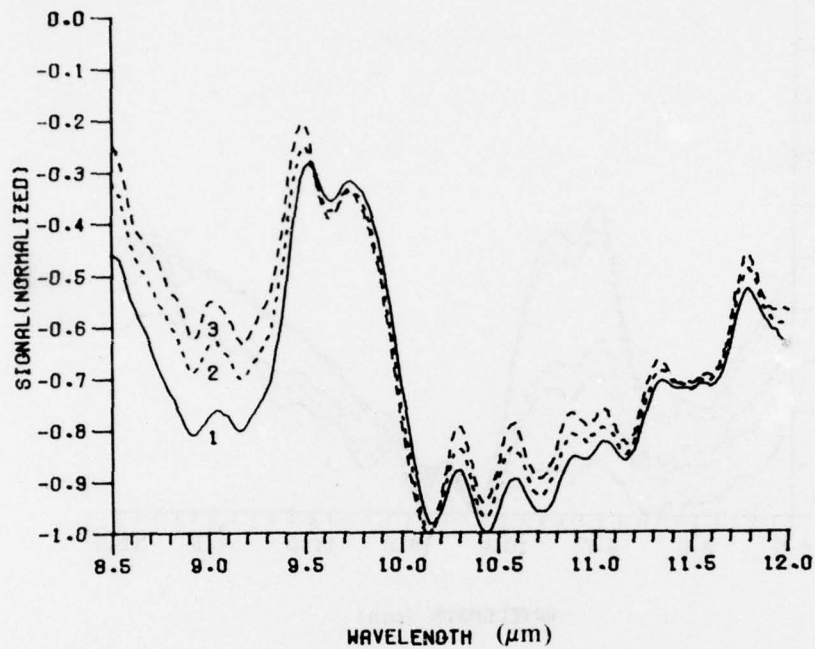


Figure 5. Two Spectra of Unknown Origin and Their LAS Background

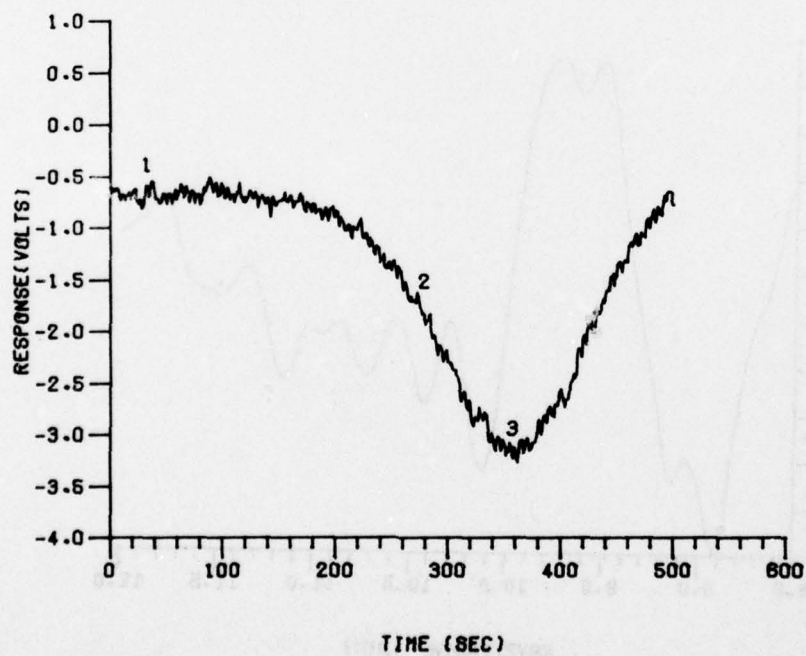


Figure 6. Negative Response from Spectra of Unknown Origin

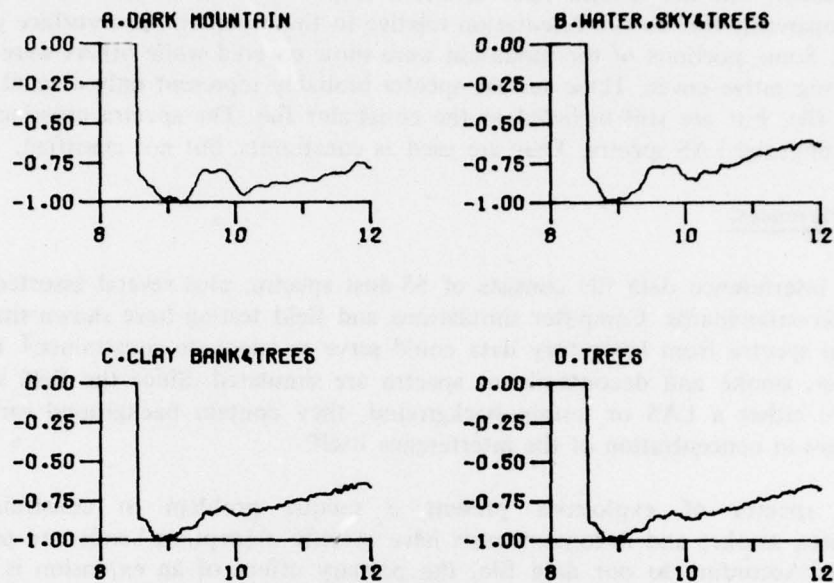


Figure 7. Four Terrain Spectra

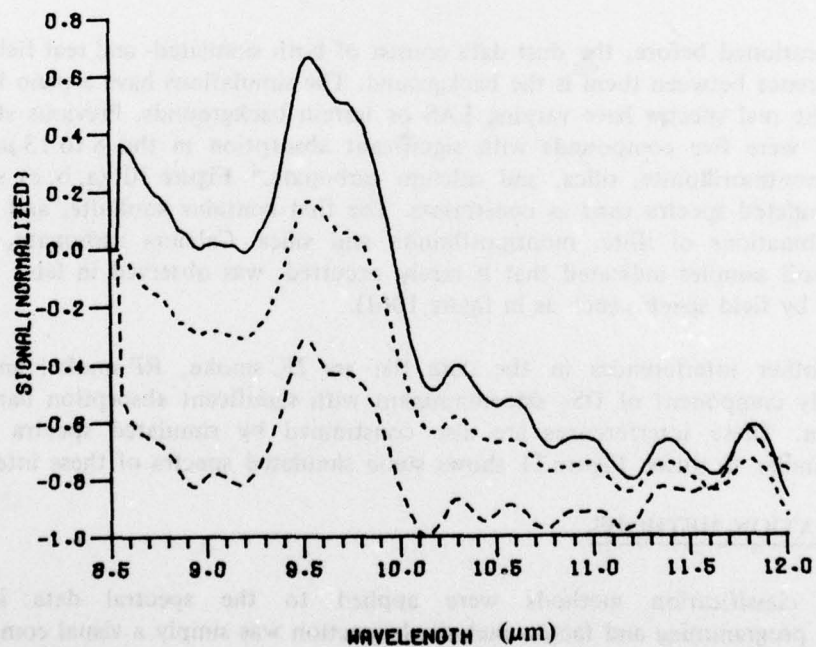


Figure 8. Spectral Variations of a Snow-Capped Mountain Range

component is present, but the spectra have different slopes and two of them cross zero. The differences are apparently due to sun orientation relative to the mountain, and surface properties of the mountain. Some portions of the mountain were snow covered while others were bare. No surface had any vegetative cover. These terrain spectra probably represent only a small part of a necessary design file, but are still included in the constraint file. The spectra crossing zero are treated like the abnormal LAS spectra. They are used as constraints, but not classified.

B. Interferences.

The interference data file consists of 55 dust spectra, plus several assorted smokes, explosions and decontaminants. Computer simulations and field testing have shown that the use of simulated field spectra from laboratory data could serve as adequate constraints.³ Therefore, many of the dust, smoke and decontaminant spectra are simulated. Since the field spectra of interferences have either a LAS or terrain background, they contain background variations in addition to changes in concentration of the interference itself.

The spectra of explosions present a unique problem in constraining and classification. Dusts, smokes and decontaminants have specific absorption bands and predictable spectral structure. According to our data file, the primary effect of an explosion is a sudden heating of air in the instrument's field of view (FOV), usually resulting in a totally saturated positive spectrum with no structure. Intermediate spectra before and after saturation are distorted, with apparently random structure (figure 9). Therefore, present data indicate that explosions produce unpredictable spectral features that cannot be classified into finite member groups.

As mentioned before, the dust data consist of both simulated- and real field spectra. The primary difference between them is the background. The simulations have a plain blackbody background and the real spectra have varying LAS or terrain backgrounds. Previous studies had shown that there were five compounds with significant absorption in the 8 to 13 μm region; kaolinite, illite, montmorillonite, silica, and calcium carbonate.⁴ Figure 10 (a, b, c) shows the three types of simulated spectra used as constraints. The first contains kaolinite, and the other two contain combinations of illite, montmorillonite and silica. Calcium carbonate, originally omitted because soil samples indicated that it rarely occurred, was observed in later field tests and is constrained by field spectra such as in figure 10(d).

The other interferences in the data file are HC smoke, RP smoke, and methyl cellulose, the only component of DS_2 decontaminant with significant absorption bands in the 8- to 13- μm region. These interferences are also constrained by simulated spectra and have response effects similar to dusts. Figure 11 shows some simulated spectra of these interferences.

III. CLASSIFICATION METHODS.

Four classification methods were applied to the spectral data: inspection, correlation, linear programming and factor analysis. Inspection was simply a visual comparison of spectral features. Correlation involved the calculation of a single numerical value that indicated

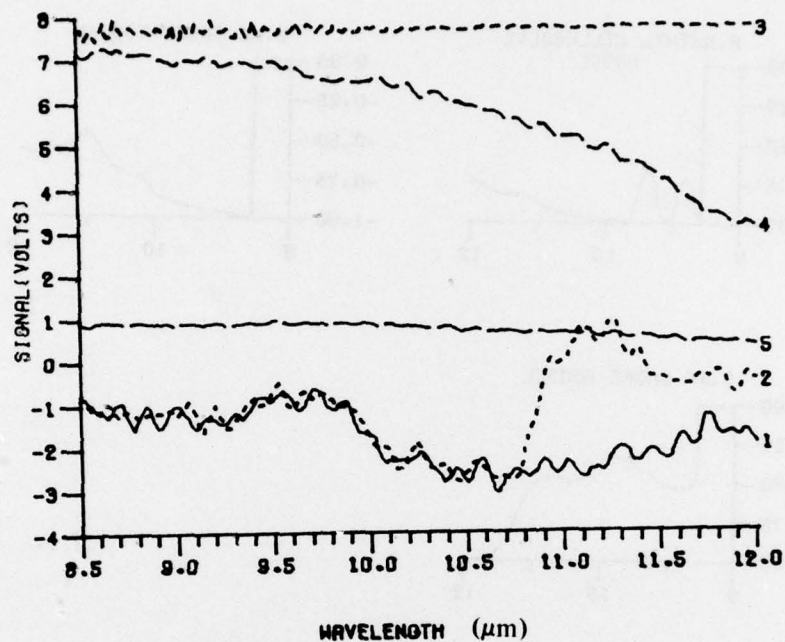


Figure 9. Explosion Sequence

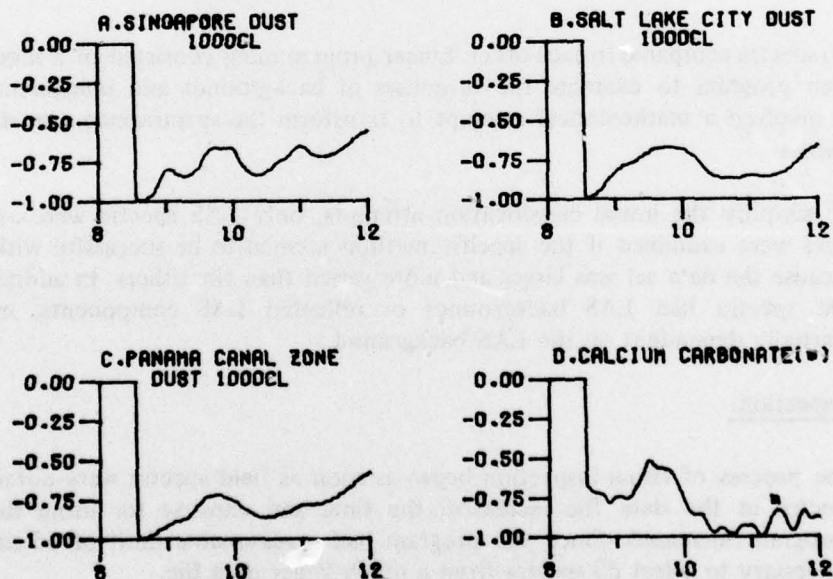


Figure 10. Four Dust Spectra

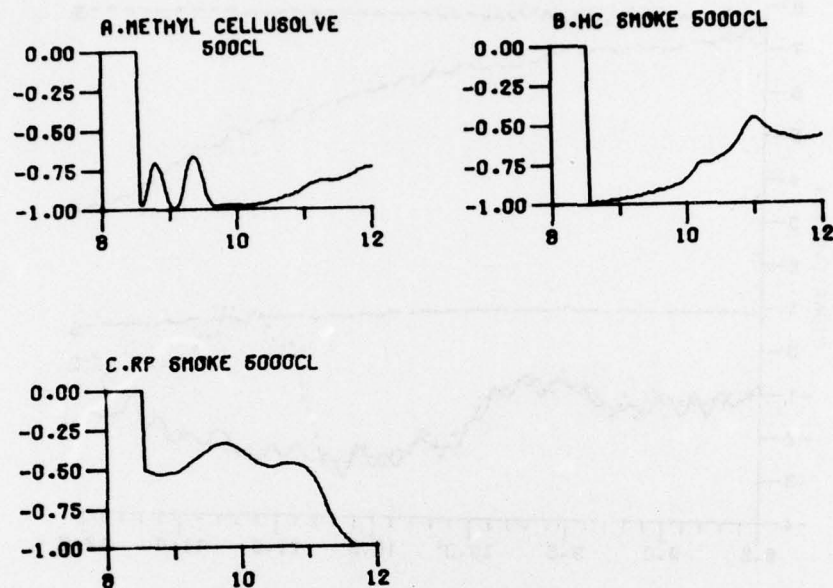


Figure 11. Three Interference Spectra

how closely two spectra compared to each other. Linear programming consisted of a modification of the optimization program to examine the responses of backgrounds and interferences. Finally, factor analysis involved a mathematical attempt to transform the spectra into a small number of significant variables.

To simplify the initial classification attempts, only LAS spectra were used. Terrains and interferences were examined if the specific method seemed to be successful with LAS. LAS was chosen because the data set was larger and more varied than the others. In addition, most of the other field spectra had LAS backgrounds or reflected LAS components, making their classification partially dependent on the LAS background.

A. Inspection.

The process of visual inspection began as soon as field spectra were obtained. As the number of spectra in the data file increased, the time and expense for using the computer optimization program increased. Since the program had a reasonable limit of 65 constraints, it soon became necessary to select 65 spectra from a much larger data file.

The selection procedure was straightforward. Spectra having approximately equal slopes and ozone intensities were compared to each other and placed in groups normally consisting of 2 to 10 spectra. One spectrum from each group, plus the individual spectra that

could not be grouped, would be added to the constraint set. For example, Figure 12 shows a group of seven spectra having similar characteristics, with the first two being nearly identical. One spectrum would be selected to represent the entire group. A set of channels and coefficients would be generated with these constraints, and the simulation program would be used to check the responses of spectra not in the constraint file.

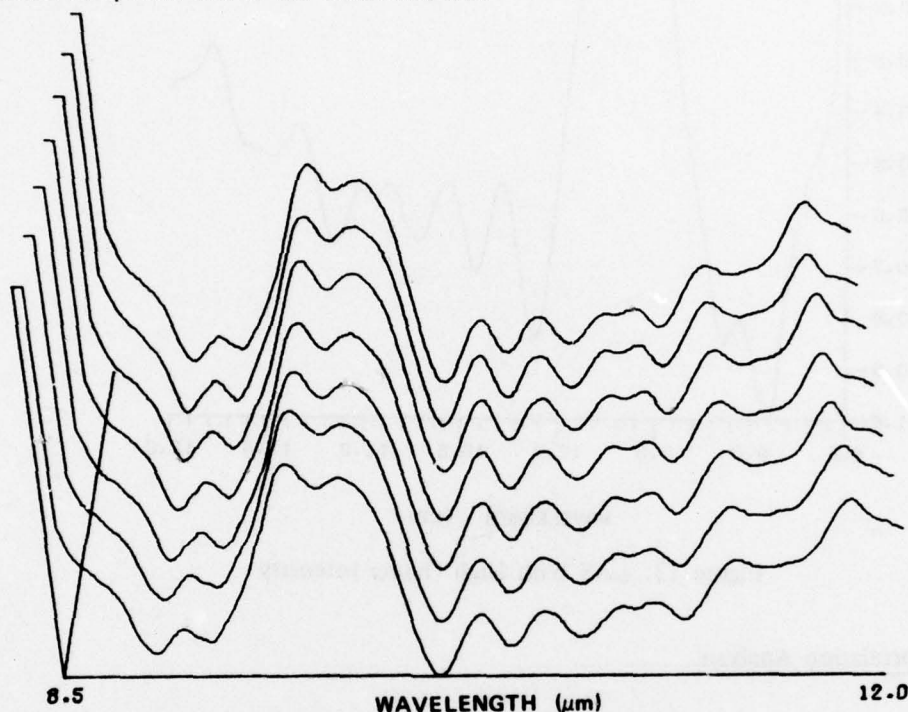


Figure 12. Similar Spectra

In the majority of cases, the technique provided adequate constraints for the existing spectral data, but there were problems. A typical solution for any set of channels and coefficients limited the constraint response to the ± 0.3 -volt range. For any set of constraints, only those spectra whose responses reached the maximum limits constrained the solution; usually 10 to 20 out of the 65. Given the same initial set, different targets had different contributing spectra. Examination of 16 different solutions involving five different targets indicated that, while some spectra affected almost all the solutions (figure 13 for example), there were others that never reached ± 0.3 volts. With few exceptions, there were no visual clues to explain why a spectrum did or did not contribute to a solution. The inability to select the dominant constraint spectra visually for any target placed a severe limitation on the utility of visual inspection. For newly obtained spectra, reliable classifications required a new spectrum to be nearly identical to one already included in the constraint file.

There were other drawbacks as well. First, the technique was basically subjective, and results could vary from person to person. In addition, the technique required all new spectra to be recorded and precisely plotted prior to classification. One of the goals of classification was to eliminate the need for recording redundant spectra. The obvious solution was to seek a mathematical technique that would be accurate, consistent, and fully automatic.

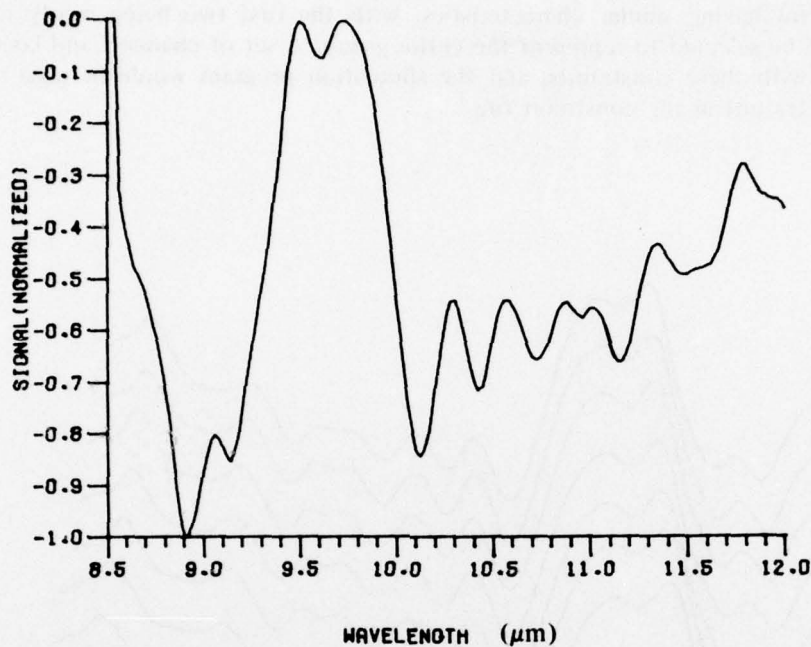


Figure 13. LAS With High Ozone Intensity

B. Correlation Analysis.

The inspection technique grouped spectra according to their spectral characteristics. This method was limited by the fact that there was no mathematical basis for the technique. Basic correlation theory provides a mathematical technique of comparing two functions dependent on the same parameter.⁵ Given two spectra, the calculation of the correlation coefficient produces a single numerical value for the degree of similarity between them.

1. Theory.

A spectrum can be represented by an N-dimensional vector where N is the number of spectral intervals. Given two spectra with signal values x_i and y_i , the vector representations are

$$\mathbf{X} = \sum_{i=1}^N \mathbf{e}_i x_i \text{ and } \mathbf{Y} = \sum_{i=1}^N \mathbf{e}_i y_i$$

where

\mathbf{e}_i is the unit vector

From vector algebra, the dot product is given by

$$\mathbf{X} \cdot \mathbf{Y} = \sum_{i=1}^N x_i y_i \quad (1)$$

The lengths of the vectors are

$$|\mathbf{X}| = X = \left(\sum_{i=1}^N x_i^2 \right)^{1/2} \quad \text{and} \quad |\mathbf{Y}| = Y = \left(\sum_{i=1}^N y_i^2 \right)^{1/2} \quad (2)$$

The ratio of the dot product to the product of the lengths is the direction cosine of the angle between them. In this case

$$\cos \alpha = \frac{\mathbf{X} \cdot \mathbf{Y}}{X Y} \quad (3)$$

By definition, $\cos \alpha$ is the correlation coefficient.

Since the dot product of two vectors is less than or equal to the product of the lengths, it is clear that the absolute value of the correlation coefficient is less than or equal to 1.

Letting K represent the correlation coefficient and applying equations (1-3) gives the following easily calculated expression⁵

$$K = \cos \alpha = \frac{\sum_{i=1}^N x_i y_i}{\left(\sum_{i=1}^N x_i^2 \right)^{1/2} \left(\sum_{i=1}^N y_i^2 \right)^{1/2}} \quad (4)$$

In applying correlation to the spectral data file, the values x_i and y_i are the signals of two spectra at .01 μm intervals from 8.68 to 11.83 μm . The correlation coefficient can assume any value from 1 to -1. Identical spectra will have correlations of 1, extremely noisy spectra could have correlations approaching 0, and two spectra having hot and cold backgrounds of equal difference energy would have a correlation of -1.

2. Results.

A computer program was written to calculate the correlation coefficients for an array of up to 72 spectra. The program operator had the option of selecting either a numerical table or a plot of the correlation of any spectrum with the other 71 in the array. In addition, other spectra not in the original array could be correlated without changing the original group.

When correlation analysis began, there were 59 LAS spectra in the data file. All were placed into an array, and correlation coefficients calculated showing the relationship of each spectrum with every other one in the array. The coefficients for these spectra ranged from 1.0000 (figure 14) to 0.8991 (figure 15).

The next step was to establish the relationship between the response difference and the correlation coefficient for two spectra. Since the normal constraint response limit was ± 0.3 volts, response values for existing sets of channels and coefficients were examined to find the lowest correlation value that would still correspond to a response difference within ± 0.3 volts. This value was empirically determined to be 0.9998. Thus, if two spectra had a correlation value of 0.9998 or greater, they would be considered the same constraint.

Having established the criterion for correlation, some questions had to be answered concerning its interpretation and effectiveness. The first question was whether or not the correlation values alone could be used to select a set of LAS spectra that would effectively constrain the entire group. A listing was made of the 59 LAS spectra. The correlation values for each spectrum were examined and all other spectra that correlated to within 0.9998 or better were listed next to that spectrum. When this was completed, the list was examined to find the least number of spectra that would constrain the entire group. A set of 29 were chosen, and using DMMP as a target, channels and coefficients were computed for this constraint set. The solution was then applied to the simulation program to obtain response values for the other 30 spectra. In every case, the responses of the unconstrained spectra were within ± 0.3 volts of their respective constraints. This result was expected because of the similarity between groups selected visually and groups selected by correlation. The advantage of the correlation method was in having a mathematical basis for the selection process.

At this point, it was obvious that given the proper hardware, the correlation technique could be used to monitor spectra automatically during field tests and eliminate those that were similar to existing constraints. However, many of the problems that occurred in visual analysis were occurring in correlation analysis. As mentioned before, for any discriminant function there existed a few dominant spectra: 7 out of 29 for this constraint set. According to their correlation values these seven spectra were expected to constrain only 17 spectra, not all 59 in the data file. From a visual standpoint there was nothing unusual about these seven spectra and correlation analysis provided no additional information. Another problem occurred when correlation values for series of spectra, such as in figure 1, were compared to their respective responses. Using the highest ozone spectrum as a base, correlation values decreased continuously in going from the highest to the lowest ozone intensity. With one exception, responses values for various sets of channels and coefficients were neither continuously decreasing nor continuously increasing. Thus, given a spectrum in the middle of a series, its response could not be estimated from its correlation value and the responses of the other spectra.

The final step in the correlation approach was to apply the technique to the set of interference spectra. An obvious shortcoming occurred when the technique was used with simulated spectra. Field spectra that had been constrained by simulated spectra did not correlate with them. As a result, the technique could not be used with simulated spectra, and thus had very limited application for interference testing.

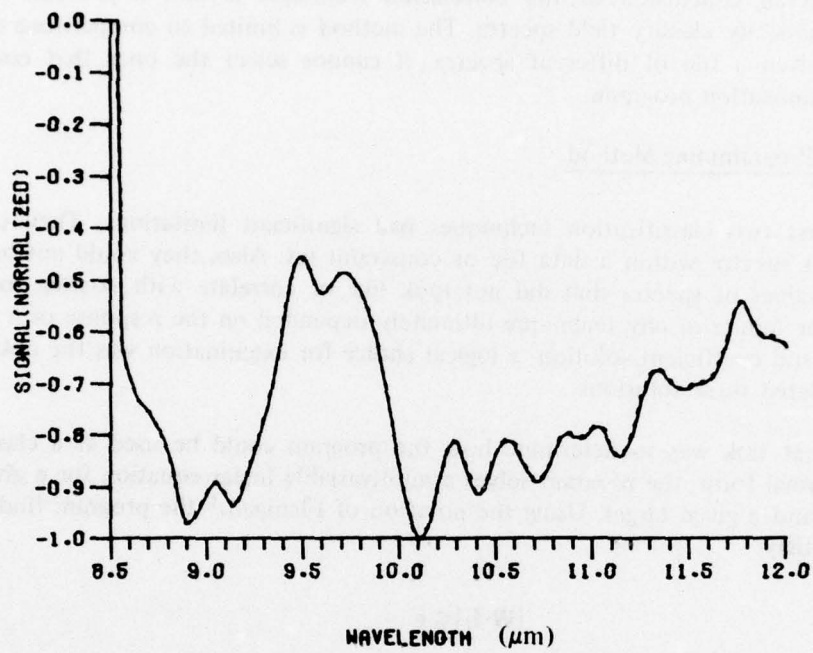


Figure 14. LAS Spectra with Correlation Value of 1.0000

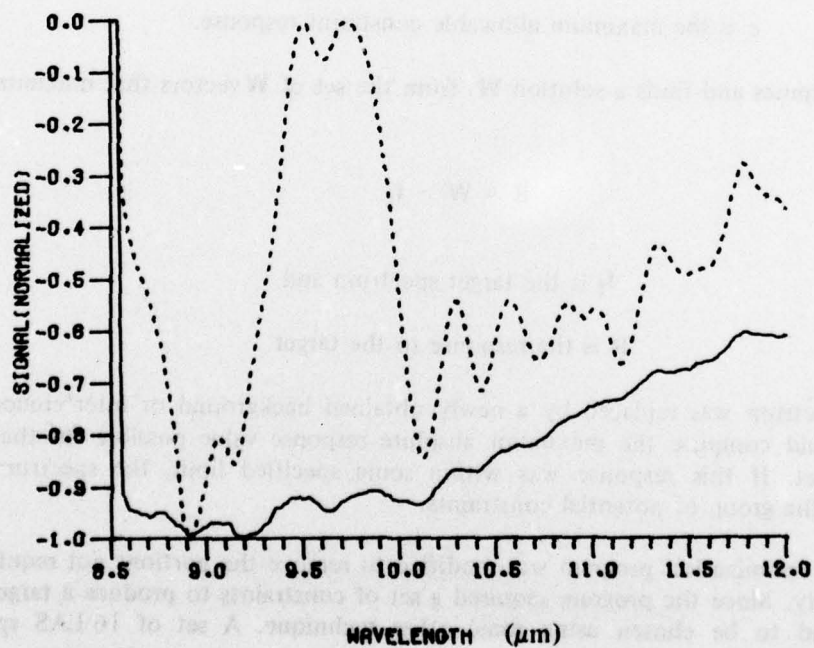


Figure 15. LAS Spectra with Correlation Value of 0.8991

The overall conclusion of the correlation technique is that it provides a limited capability to automatically classify field spectra. The method is limited to comparisons of nearly identical spectra. Given a file of different spectra, it cannot select the ones that control the solutions of the optimization program.

C. Linear-Programming Method.

The first two classification techniques had significant limitations. They could not select the dominant spectra within a data file or constraint set. Also, they could not be used to estimate response values of spectra that did not look like or correlate with existing constraints. Since the success or failure of any technique ultimately depended on the response of a spectrum to a given channel and coefficient solution, a logical choice for examination was the optimization program that calculated these solutions.

The first task was to determine how the program could be used as a classification method. In its normal form, the program solves a multivariable linear equation for a given set of constraint spectra and a given target. Using the notation of Flanigan,¹ the program finds a set of vectors \mathbf{W} which satisfy

$$|\mathbf{W} \cdot \mathbf{f}_j| \leq \epsilon$$

where

the \mathbf{f}_j are linearly independent constraint spectra and

ϵ is the maximum allowable constraint response.

The program continues and finds a solution \mathbf{W}' from the set of \mathbf{W} vectors that maximizes

$$R = \mathbf{W}' \cdot \mathbf{f}_t$$

where

\mathbf{f}_t is the target spectrum and

R is the response to the target.

If the target spectrum was replaced by a newly obtained background or interference spectrum the program would compute the maximum absolute response value possible for that spectrum and constraint set. If this response was within some specified limit, the spectrum could be eliminated from the group of potential constraints.

The optimization program was modified to remove the portions not required for the classification study. Since the program required a set of constraints to produce a target response, an initial set had to be chosen using some other technique. A set of 16 LAS spectra were

selected based on physical characteristics. This initial selection required subjective judgements that would be acceptable provided the rest of the program produced decisive results.

The most difficult step was determining the response criterion for the elimination of spectra. Spectra not included in the constraint set would probably have maximum response values that were outside the normal range of ± 0.3 volts. The new limit had to be high enough to eliminate common spectra but low enough to prevent the elimination of significant spectra. A value of three times the normal constraint limit was chosen as the maximum-allowed-response range. This meant that a spectrum eliminated by this method could have as much as a ± 0.9 -volt response for a solution designed to detect an agent. However, the actual response of a spectrum to a solution calculated for an agent was expected to be much less than the maximum-allowed-response value.

The classification procedure was simple. Starting with the basic constraint set, the remaining 70 LAS spectra (27 more had been added since the correlation study) were inserted individually as target spectra in the modified program. If the response of the spectrum exceeded ± 0.9 volts, it was added to the constraint set and the process continued with the enlarged constraint set and remaining spectra.

The response values obtained from this procedure were larger than anticipated. It was hoped that most of the spectra would have responses close to the normal range of ± 0.3 volts, and that a few would have much higher responses that exceeded the ± 0.9 -volt range. In fact, only 6 of the 70 spectra had responses within ± 0.6 volts and 37 had responses exceeding ± 0.9 volts; almost the opposite of the desired result. Thus, a total of 53 constraints was required from the data file of 86 LAS spectra. From a percentage basis, this number of constraints was too large to allow expansion of the method to the entire data file. Some thought was given to increasing the maximum-allowed response, but the potential decrease in the number of constraints would have been offset by a decrease in the reliability of the method. Procedural changes were also considered, but none appeared likely to make any significant improvement.

These results indicated that the linear-programming technique was unsuitable for classification purposes. The technique required subjective judgements to initiate the classification process, and thus required that the resulting response values be capable of clearly defining the significant spectra in the data file. The actual response values did not produce decisive results, and reliable classifications could not be obtained. Nevertheless, the technique provided some essential information concerning the effectiveness of classification methods.

All of the classification techniques rely on a basic assumption that two spectra from a data set can be used to constrain a third spectrum not included in that set. This assumption was supported by field tests and computer simulations. The results of the linear-programming attempt at classification indicated that this assumption might not always be valid. Since most of the spectra eliminated by this method had responses between 0.6 and 0.9 volts, there was at least that one solution in which these spectra would not be adequately constrained to ± 0.3 volts by the constraint file. There was no guarantee that other problem solutions did not exist and that some future agent solution might not have a false alarm if one of these so-called insignificant

spectra were encountered. This latter problem could exist for any spectrum eliminated as a constraint by any classification method. The experience to date indicates that it is unlikely to occur, but any future work should examine this problem in more detail.

D. Factor Analysis.

The first three classification techniques had very limited success. None of them were able to select the significant spectra from a data file and reduce the number of constraints to a workable level. When applied to the entire data set, at least 100 spectra would have been required as constraints by each of the methods. In addition, each of the methods required subjective judgements to select some of the constraints. Any new technique should eliminate the subjective choosing of constraints, isolate the significant spectra or the significant features within a given spectrum, and provide all the information required to pick suitable constraints.

1. Theory.

Factor analysis is a procedure to find a new set of variables (called factors) which describe a set of data.⁶ In this case, the data are a collection of spectra with common characteristics. Each spectrum consists of a signal measured at N different wavelengths and can be treated as an N -component vector \mathbf{s}_j where the subscript designates a particular spectrum in the collection.

$$\mathbf{s}_j = \begin{pmatrix} s_{1j} \\ s_{2j} \\ \vdots \\ s_{Nj} \end{pmatrix} \quad j = 1, 2, \dots, n$$

s_{ij} is the signal of the j^{th} spectrum measured at the i^{th} wavelength. There are n spectra in the collection.

The first step in factor analysis is to convert the raw data to a standardized form in order to simplify the mathematics. At each wavelength, the average signal \hat{s}_i and the variance σ_i^2 are computed from

$$\hat{s}_i = \frac{1}{n} \sum_{j=1}^n s_{ij} \quad i = 1, 2, \dots, N$$

$$\sigma_i^2 = \frac{1}{n} \sum_{j=1}^n (s_{ij} - \hat{s}_i)^2$$

The raw data variables S_{ij} are then transformed to standardized variables

$$Z_{ij} = \frac{1}{\sigma_i} \left(S_{ij} - \bar{S}_i \right)$$

Standardized vectors Z_j , each representing a particular spectrum, may be combined into a matrix Z containing all the spectra in the collection. Each column of Z is one spectrum while each row represents a specific wavelength. The size of Z is $N \times n$.

The fundamental assumption of factor analysis is that each standardized variable Z_{ij} can be written as a linear combination of new variables or factors. The factors are considered to be hypothetical constructs whose general nature is unknown but which can be calculated for a specific case. The number of factors needed to reproduce the original data exactly is equal to the number of original data variables. In practice, it is usually possible to reconstruct the original data to an acceptable degree of accuracy with a smaller number of factors. The basic model of factor analysis can be written as

$$Z_i = \sum_{k=1}^m \alpha_{ik} f_k \quad (5)$$

Each Z_i is the standardized signal at the i th wavelength for an arbitrary spectrum. A total of m factors f_k are being used. The α 's are constants and α_{ik} is called the loading of factor k on variable i . The loadings are correlations between the original variables and the factors, and are found, as shown below, from the eigenvalues and eigenvectors of the data correlation matrix R .

Once the matrix Z of standardized data has been constructed, it is an easy matter to calculate the correlation matrix R since

$$R = \frac{1}{N} Z Z' \quad (6)$$

The prime denotes the transposition of the matrix. The matrix R is square and symmetric with 1's along the main diagonal. Each element r_{ij} is the statistical correlation between standardized variables Z_i and Z_j .

As mentioned above, the loadings are derived from the eigenvalues and eigenvectors of R . Techniques for finding eigenvalues and eigenvectors can be found in reference 7. Let $\lambda_1, \lambda_2, \dots, \lambda_N$ be the eigenvalues such that $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_N$ and V_1, V_2, \dots, V_N the corresponding eigenvectors. The loadings may be found from

$$\alpha_{ik} = \frac{\sqrt{\lambda_k} V_{ik}}{\sqrt{\sum_{j=1}^N V_{jk}^2}} \quad i = 1, \dots, N, \quad k = 1, \dots, N$$

The number m of factors to be used for a given set of data can be determined from the eigenvalues. The ratio

$$\frac{\sum_{j=1}^m \lambda_j}{\sum_{j=1}^N \lambda_j} \quad (7)$$

is the proportion of the variation in the data reproduced by the m factors.

The α 's may be combined into an $N \times m$ matrix \mathbf{A} . The basic model of factor analysis may now be written as

$$\mathbf{Z} = \mathbf{A} \mathbf{F} \quad (8)$$

where \mathbf{F} is the matrix of factor scores.

Substituting equation (8) into equation (6) and using the fact that the transposition of the product of two matrices is equal to the product of their transpositions in reverse order, one obtains

$$\mathbf{R} = \mathbf{A} \left[\frac{\mathbf{F} \mathbf{F}'}{N} \right] \mathbf{A}'$$

The quantity in parenthesis is the dot product of a set of orthogonal vectors with itself and is therefore equal to the identity matrix. The result is called the fundamental equation of factor analysis.⁸

$$\hat{\mathbf{R}} = \mathbf{A} \mathbf{A}' \quad (9)$$

The circumflex signifies that this $\hat{\mathbf{R}}$ is the matrix of reproduced correlations. In general, it will be identical with the original correlation matrix \mathbf{R} only if N factors are used. Comparison of $\hat{\mathbf{R}}$ and \mathbf{R} shows the extent to which the number of factors used in the calculation accurately reproduces the original data.

Another useful matrix equation can be obtained by considering the product of \mathbf{A}' and \mathbf{A} . Using several theorems from linear algebra, it can be shown that

$$\Lambda = \mathbf{A}' \mathbf{A} \quad (10)$$

where Λ is a diagonal matrix whose diagonal elements are the eigenvalues λ_i .⁷ The size of Λ is $m \times m$.

It is possible to generate a more useful set of loadings by forming linear combinations of the original loadings. The new loadings are referred to as rotated loadings while the original loadings are described as unrotated loadings. The names are derived from the procedure for calculating the new loadings which consists of a series of rotations in an m -dimensional vector space. The rationale for calculating a new set of loadings stems from the manner in which the different sets of loadings correlate with the original variables. The unrotated loadings generally have a high correlation with many of the original variables while the rotated loadings correlate highly with just a few variables. It should be easier to gain insight into the relationship between the original variables which have a high correlation with a rotated loading because of the smaller number of variables.

Although many procedures exist for calculating the rotated loadings the Kaiser Varimax method as described in references 6 and 8 was used. The matrix of rotated loadings \mathbf{B} is computed from \mathbf{A} by an orthogonal transformation matrix \mathbf{T} .

$$\mathbf{B} = \mathbf{A} \mathbf{T} \quad (11)$$

In terms of the rotated loadings, the basic model of factor analysis may be written as

$$\mathbf{Z} = \mathbf{B} \mathbf{F}_R \quad (12)$$

The subscript on \mathbf{F}_R identifies the rotated factors which are different from the unrotated factors \mathbf{F} .

Even though the general nature of the factors is unknown, specific values of each factor can be calculated for a given \mathbf{Z}_j . These numbers are referred to as factor scores. A set (vector) of factor scores \mathbf{F}_{Rj} is computed for each standardized signal \mathbf{Z}_j and is used to classify each signal. The size of \mathbf{F}_{Rj} is $m \times 1$. Premultiplying (12) by $(\mathbf{B}' \mathbf{B})^{-1} \mathbf{B}'$, the factor scores can be found from

$$F_{Rj} = B'B^{-1}B'Z_j$$

Unfortunately, it is usually not practical to use equation (13) to calculate the factor scores because it is necessary to use the full $N \times N$ matrix for B when computing the inverse. This means that all N loadings must be found and rotated. It would be preferable to perform the calculation by use of only m loadings. This accomplished with the following equation which is derived in appendix A.

$$F_{Rj} = B'A \Lambda^{-2} A'Z$$

2. Results.

A computer program was written to calculate all the required parameters needed to produce a set of rotated loadings and corresponding factor scores for data sets of up to 200 spectra. Computer subroutines from the International Mathematical and Statistical Libraries, Inc. were used to calculate A , B and $T9$. The program's output included listings of variances, eigenvalue ratios and factor scores, plus plots of the mean spectrum, standard deviation, loadings, and reconstructed spectra. There was no preconceived idea as to what the results would be or how they would be used for classification. It was hoped that the data would be reduced to a small group of factors and loadings that represented the most significant spectral properties.

As before, the technique was first applied to the set of LAS spectra. The program divided the spectra into 63 intervals of $0.05 \mu m$ from 8.68 to $11.83 \mu m$, the same as in the optimization program. This meant that a maximum of 63 loadings and factor scores would be required to reproduce a spectrum. The first step was a quick calculation of the eigenvalue ratios for the first 20 factors (expression 7). The cumulative percentage value in table 1 is the eigenvalue ratio and represents the proportion of variation reproduced by the number of factors; thus, the first 20 out of 63 factors were responsible for 99.98% of the variation. Clearly as the number of factors increases, the importance of the individual factor to the reconstruction decreases. Ten factors were chosen for the initial classification attempt, and rotated loadings and factor scores were calculated for the 86 LAS spectra.

Table 1. Eigenvalues and Eigenvalue Ratios for the First 20 Factors from the LAS Data File

Factor number	Eigenvalue	Cumulative percentage	Factor number	Eigenvalue	Cumulative percentage
1	32.6060	51.76	11	.0128	99.92
2	24.2045	90.18	12	.0099	99.93
3	3.2292	95.30	13	.0065	99.94
4	2.1455	98.71	14	.0049	99.95
5	.3619	99.28	15	.0046	99.96
6	.1687	99.55	16	.0038	99.96
7	.0971	99.70	17	.0028	99.97
8	.0605	99.80	18	.0026	99.97
9	.0382	99.86	19	.0020	99.98
10	.0234	99.90	20	.0018	99.98

At this point, the resulting data are examined in an attempt to apply them to the classification study. As mentioned before, the loadings are correlations between the original variables and the factors. The plots of the rotated loadings (figure 16) showed decreasing correlation values with an increase in factor number, again verifying the decreasing significance of higher order factors. The factor scores themselves consisted of positive and negative numbers ranging from -3.8

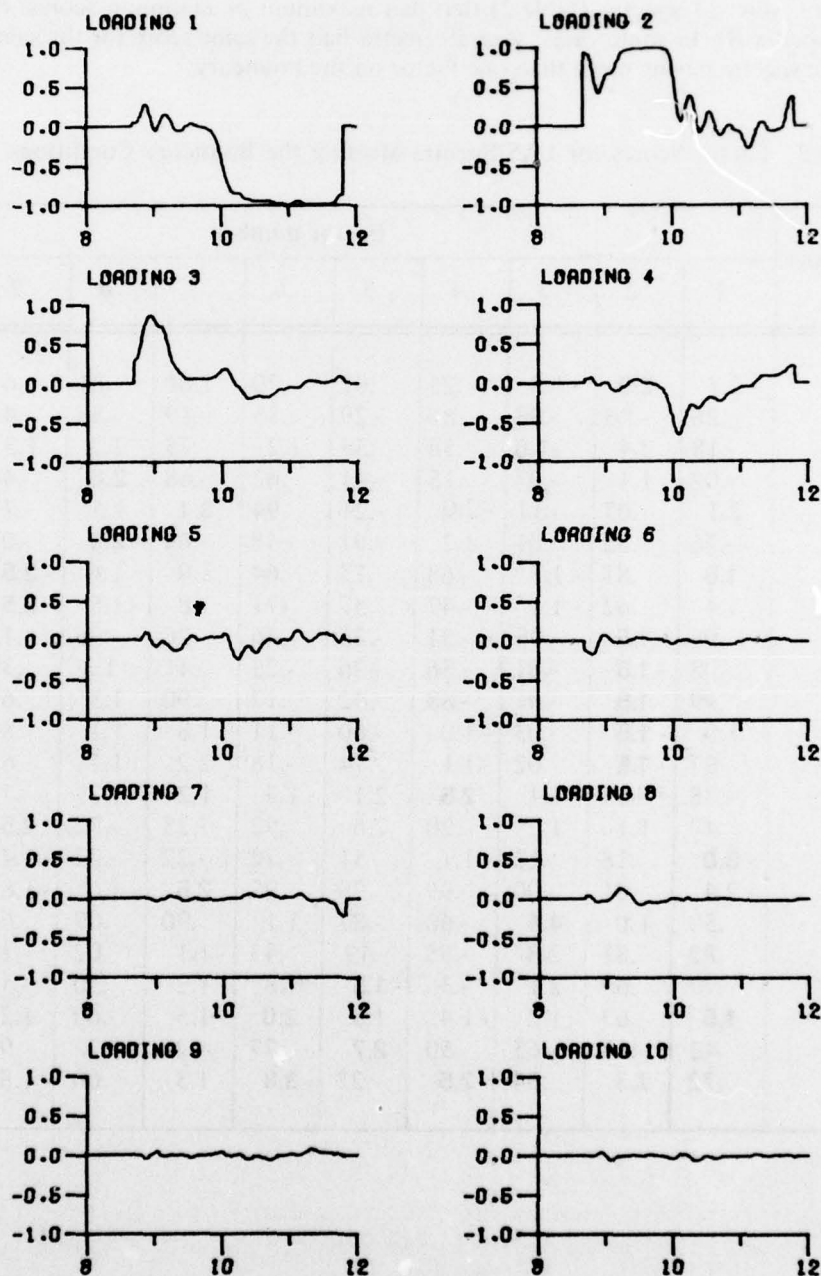


Figure 16. First 10 Rotated Loadings from LAS Data File

to +5.5 for the 86 LAS spectra. An assumption was made that the maximum and minimum scores for each factor might create a boundary condition for the data set. Those spectra having one or more factors on the boundary might be the most significant spectra in the data file, and as such, would be constraint candidates. Such a selection would be entirely based on numerical data and would not require any subjective judgements.

There were 23 spectra (table 2) that had maximum or minimum scores. (Spectra are illustrated in appendix B). In some cases, several spectra had the same score for the same factor; in others, there were spectra having more than one factor on the boundary.

Table 2. Factor Scores for LAS Spectra Meeting the Boundary Conditions

Spectrum number	Factor number									
	1	2	3	4	5	6	7	8	9	10
1	-1.7	2.9	-1.3	.25	.01	-.70	1.00	.81	1.6	-2.6
2	-.20	-.76	-.08	.86	-.29	.55	-.19	-.89	-.45	-2.6
3	-.18	2.4	-1.6	.58	.38	1.2	.75	2.2	1.3	-1.4
4	-.02	1.1	-.97	.15	-.41	.62	-.68	2.6	.44	.10
5	-2.1	.07	-.11	-2.0	-.21	.94	3.1	-1.5	-.77	-.16
6	-.76	-.52	-.01	1.2	-.91	-.48	-.64	-2.6	-.07	-.62
7	1.5	.81	-1.3	-.68	.73	.64	1.9	-1.6	-2.5	-.22
8	1.4	.62	-1.1	-.47	.59	.71	1.8	-1.5	-2.5	-.18
9	.98	-1.5	-.06	-.31	-.28	-.46	.26	.96	.13	-.04
10	.98	-1.5	-.01	-.56	-.26	-.25	.41	1.3	.35	-.10
11	.99	-1.5	-.01	-.88	-.42	.17	.90	1.5	.64	-.46
12	1.0	-1.5	-.05	-1.0	-.60	-.11	1.8	1.1	.89	.01
13	.97	-1.5	.02	-1.1	-.74	-.18	2.2	1.1	.61	.76
14	-.75	-.43	1.4	2.5	2.1	-1.3	1.2	1.7	-.72	2.2
15	.47	1.1	1.2	.20	2.6	.92	-.25	-.72	2.5	-1.5
16	-3.0	.18	.12	-1.1	.51	.72	-.22	-.22	-1.4	.09
17	-2.4	.01	-.00	-.99	.98	.95	-2.5	1.6	-1.8	.38
18	.50	1.0	4.4	-.60	-.87	1.1	.90	.09	.66	.53
19	.82	.81	2.8	-.85	-.49	.43	-1.1	.02	-.19	-2.6
20	.79	.69	2.1	-.36	-1.5	1.8	-1.2	.30	-.55	.69
21	1.5	.63	-1.2	-1.4	1.3	2.0	-1.5	-.60	1.2	2.2
22	.42	.68	-.65	.50	2.7	.77	-.20	-1.2	.90	.05
23	.72	2.3	.34	-2.5	-.22	-3.8	-1.3	.00	-1.8	.39

Those 23 spectra were then put into a file and used as constraints for an agent target in the optimization program. The resulting set of channels and coefficients were then used in the simulation program to obtain the responses of all the spectra. Many of the LAS spectra had responses within ± 0.3 volts. Only one LAS had a response exceeding ± 0.6 volts. These results indicated that the technique was promising. A slight increase in the number of factors might produce a reasonably sized constraint set that would constrain the entire file to within the desired ± 0.3 volts. In addition, the technique might also be applied to the entire data file with little difficulty.

A new file of 162 spectra was established that consisted of all LAS, terrain, and interference spectra except those in which part of the spectrum was positive. As before, the eigenvalues for the first 20 factors were obtained as a guide in selecting the number of factors to be used for classification. Fifteen factors, representing 99.91% of the variation were chosen. The 15 loadings, and corresponding factor scores for each spectrum were calculated. The factor scores ranged from -8.3 to +7.0 for the 162 spectra in the file. The total number of spectra having one or more boundary factor scores was 27. If these 27 proved to be capable of constraining the entire group of 162, then factor analysis would be the most promising classification technique.

Using these 27 spectra as constraints, a set of channels and coefficients were obtained. This solution was used in the simulation program to obtain response values for every spectrum in the data file. Each of the 162 spectra had response values within ± 0.6 volts, a significant result. It should be noted that in both groups of data, an eigenvalue ratio of approximately 99.91% resulted in response values within ± 0.6 volts. These results indicated that the technique should produce reasonable constraints if the number of factors was increased to obtain a higher eigenvalue ratio.

The limiting eigenvalue ratio was then increased to 99.98%, and loadings and factor scores were obtained for both the LAS file and the larger mixed file. This resulted in 19 factors and 32 constraints for the LAS file, and 27 factors and 37 constraints for the mixed file. Channel and coefficient sets for two different agents were obtained for both constraint sets, and the solutions were entered into the simulation program to obtain response values. For the LAS constraints, the remaining 54 LAS spectra were constrained to within ± 0.4 volts with the exception of five spectra from one solution and two spectra from the other. For the mixed constraints, the remaining 125 spectra were constrained to within ± 0.4 volts with the exception of three spectra from one solution and two spectra from the other. The highest response for any of the above exceptions was 0.605 volts. These results indicated that the factor analysis technique coupled with the established procedure for selecting constraints, was the most effective and reliable of the four methods examined. Given a large data file, the technique will select a reasonably sized set of spectra that will constrain the entire data file adequately to within some specified response limit. The technique is specific and requires no subjective selection of any spectra.

One final question was the ability of factor analysis to classify new spectral data. Based on the previous results, it was assumed that any new spectrum having factor scores less than the established boundary scores would be adequately represented by existing constraints. This assumption was tested by examination of five dust and five LAS spectra not included in any of the previous trials. The 27 factor scores from the mixed-constraint set were calculated for the new spectra and compared to the boundary scores. Only one spectrum, the LAS in figure 4, had factor scores exceeding the boundary limits. All 10 spectra were placed in the simulation

program and responses obtained for the two agent solutions for the larger data set. None of the new spectra had responses exceeding the ± 0.4 volt range. Basically, this supported the assumption that factor scores within the boundary implied that the spectrum was not significant; however, since the spectrum having scores outside the limit did not exceed the response range, the assumption is still uncertain. A complete answer to this question requires many more examples in order to obtain a statistical basis for the final answer.

The overall conclusion of the factor analysis study is that the technique can select a small group of representative constraints from a large data file. The method has the potential for automatic implementation and could prove to be capable of classifying new spectra in real time.

IV CONCLUSIONS.

Of the four methods examined, the factor analysis technique was the most useful and came the closest to meeting all of the original objectives. The correlation technique could be used to determine whether one spectrum was nearly identical to another spectrum, but could not make any significant reduction in the constraint file. The inspection technique was useful, but could not be automatically implemented or make a significant reduction in the number of constraints. The linear-programming technique required too many subjective judgements and was too complex to select constraints automatically. Its most useful result was to illustrate the possible limitations in any classification system.

The 37 spectra chosen as constraints from the factor analysis technique come close to meeting the requirements for a set of independent spectra and are shown in appendix C.

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APPENDIX A DERIVATION OF F_{Rj} EQUATION

Factor scores can be calculated from the unrotated and rotated loadings without computing all N loadings.*

From (8)

$$Z_j = A F_j$$

and

$$F_j = (A' A)^{-1} A' Z_j$$

Using (10)

$$F_j = \Lambda^{-1} A' Z_j \tag{A-1}$$

which is the unrotated factor score.

The rotated factor scores are a little more difficult. From (12)

$$Z_j = B F_{Rj}$$

Therefore,

$$A F_j = B F_{Rj}$$

and using (11)

$$A F_j = A T F_{Rj}$$

or

$$F_{Rj} = T' F_j \tag{A-2}$$

since T is an orthogonal matrix.

Combining A-1 and A-2,

$$F_{Rj} = T' \Lambda^{-1} A' Z_j \tag{A-3}$$

* See Literature Cited on the next page.

Using (11) again,

$$B = AT$$

$$A'B = A'AT$$

$$(A'A)^{-1}A'B = T$$

$$\Lambda^{-1}A'B = T$$

Therefore,

$$T' = B'A\Lambda^{-1} \quad (A-4)$$

Substituting A-4 into A-3, one obtains (14)

$$F_{Rj} = B'\Lambda^{-2}A'Z_j$$

The reconstructed spectrum $\overset{\Lambda}{Z}_j$ can be found from

$$\overset{\Lambda}{Z}_j = BB'A\Lambda^{-2}A'Z_j \quad (A-5)$$

LITERATURE CITED

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APPENDIX B

TEN FACTOR CONSTRAINTS

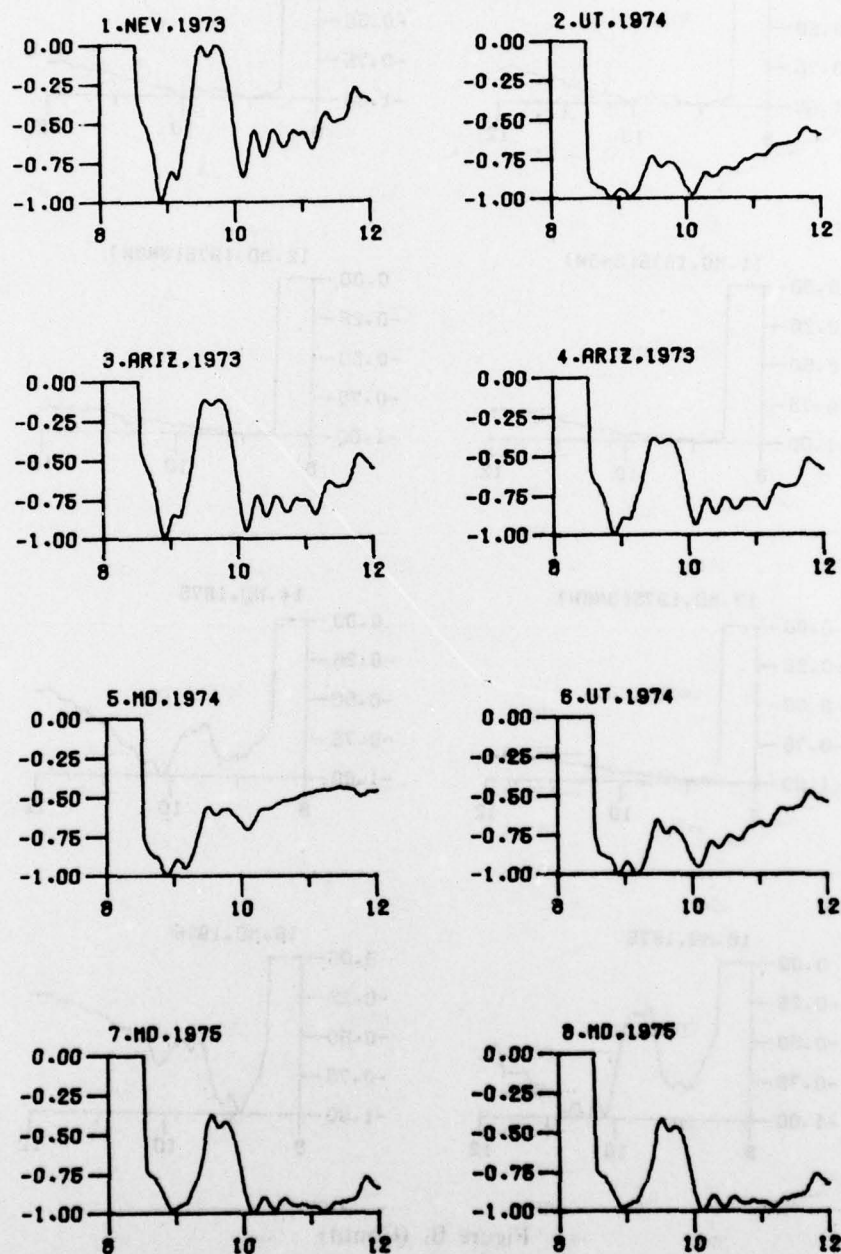


Figure B. Constraints from LAS Data File Based on Ten Factors

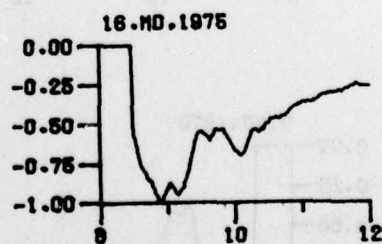
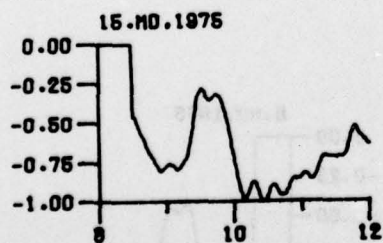
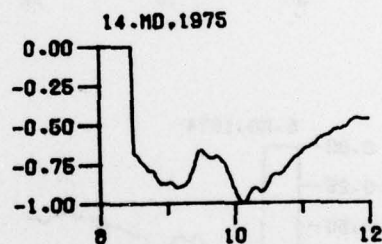
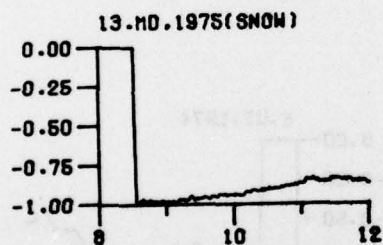
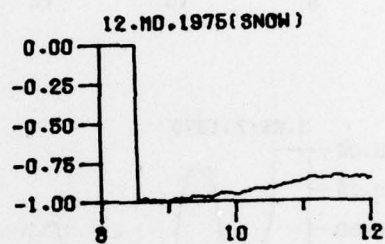
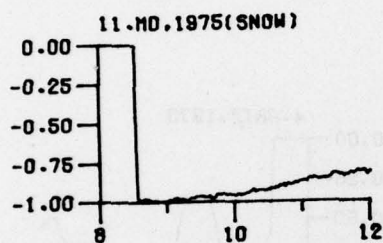
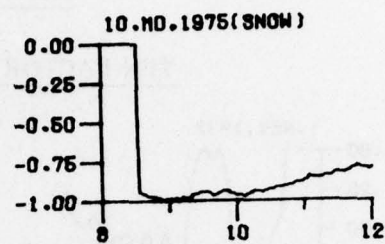
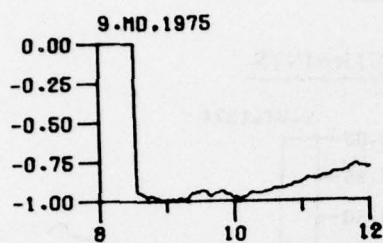


Figure B. (Contd)

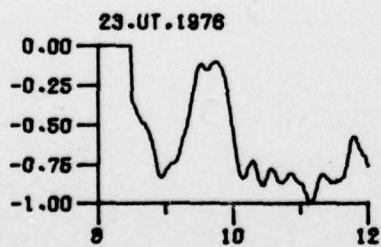
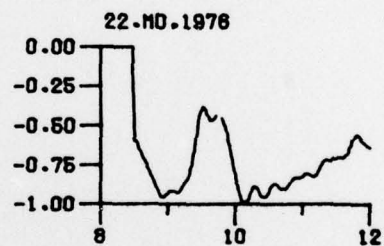
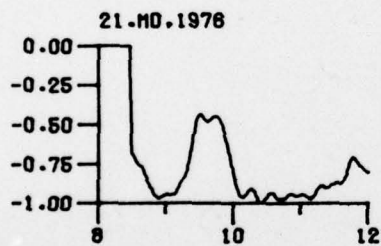
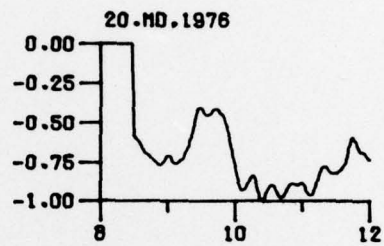
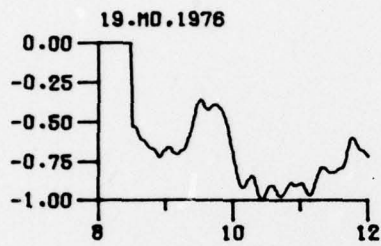
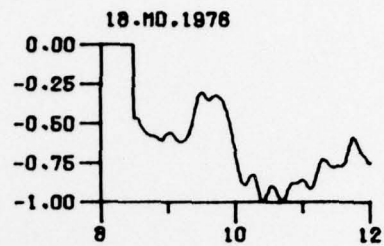
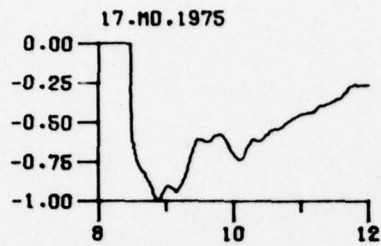


Figure B. (Contd)

APPENDIX C

THIRTY-SEVEN SPECTRA CHOSEN AS CONSTRAINTS FROM THE FACTOR ANALYSIS TECHNIQUE

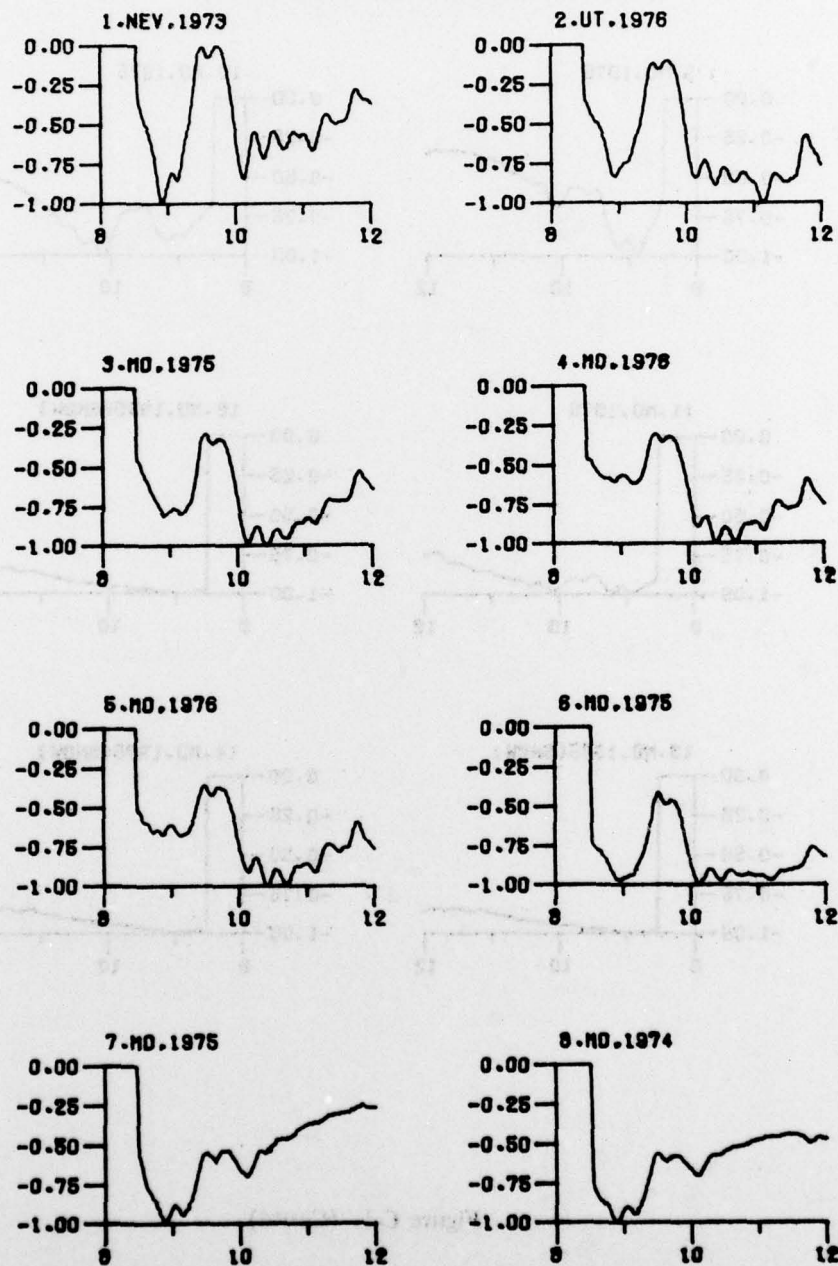


Figure C-1. LAS Constraints

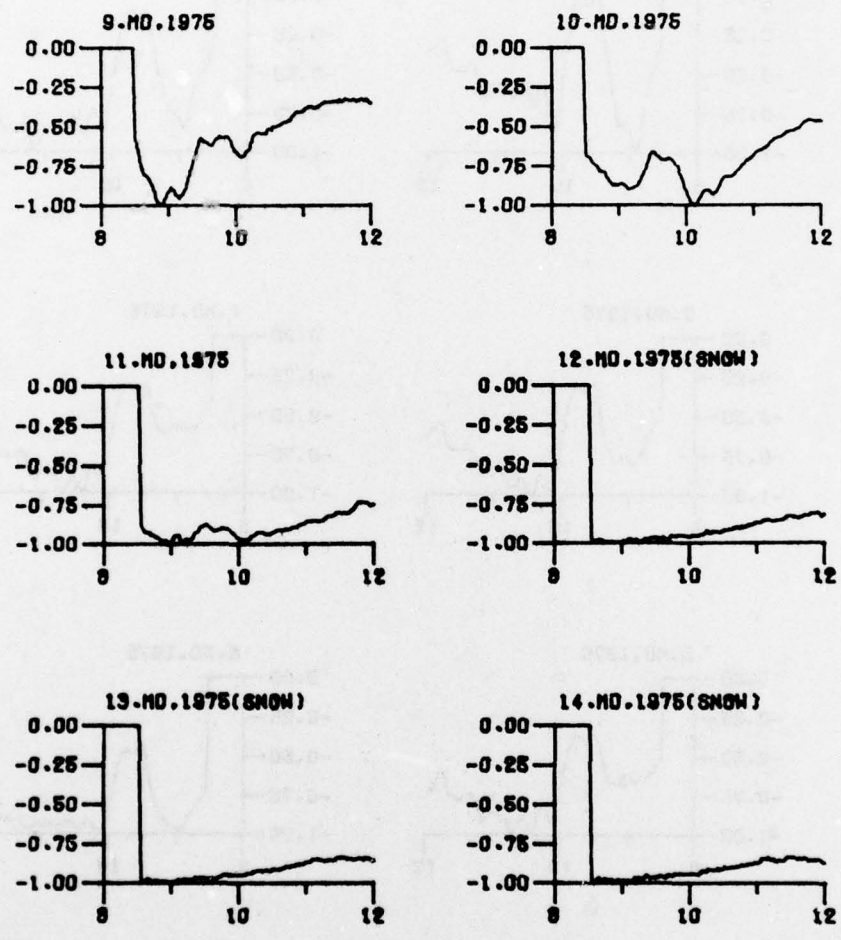


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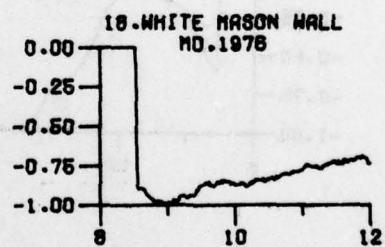
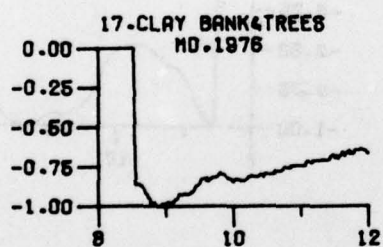
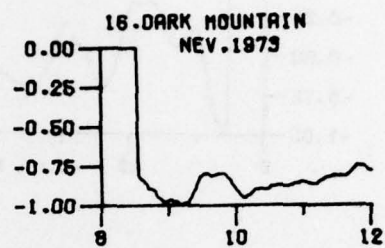
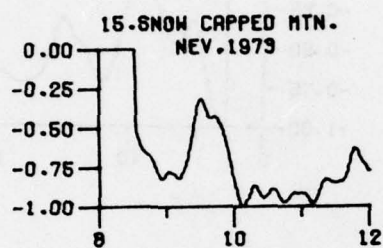


Figure C-2. Terrain Constraints

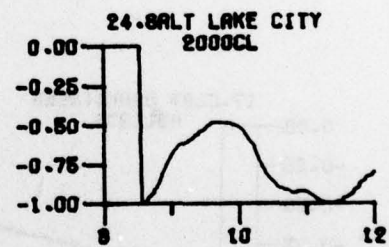
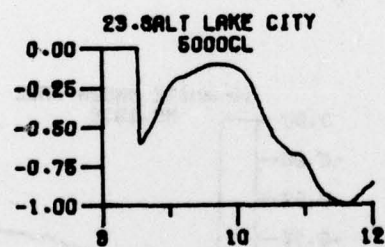
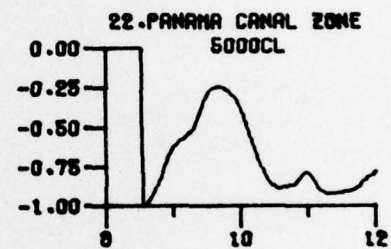
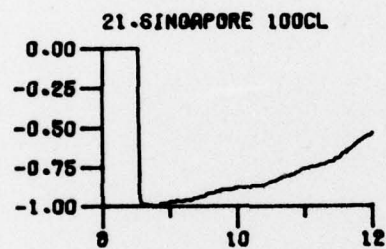
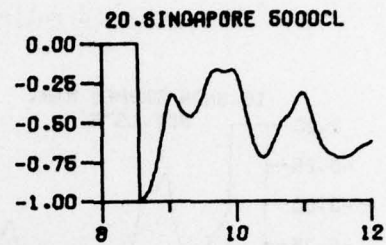
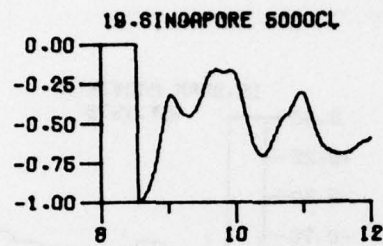


Figure C-3. LAB Simulated Dust Constraints

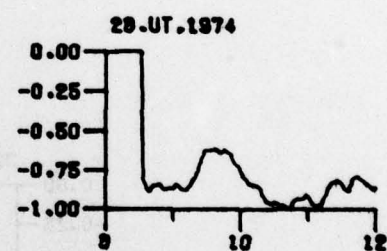
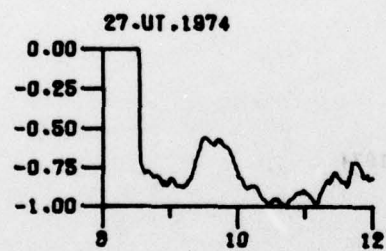
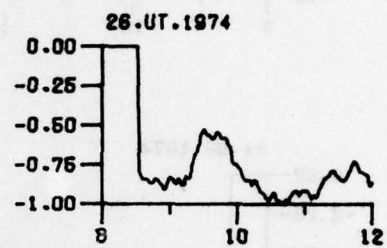
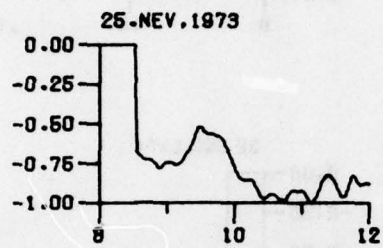


Figure C-4. Dust Constraints

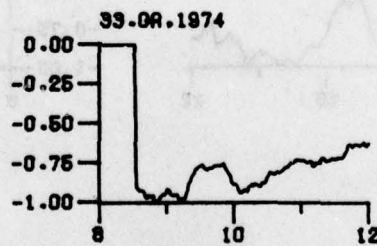
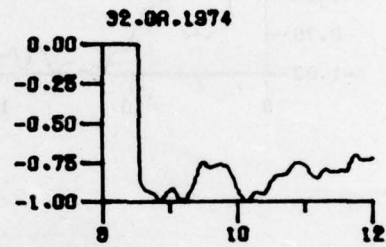
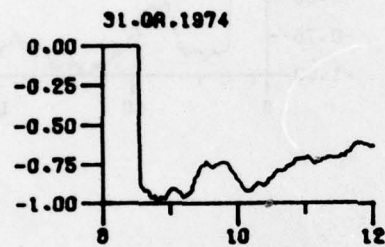
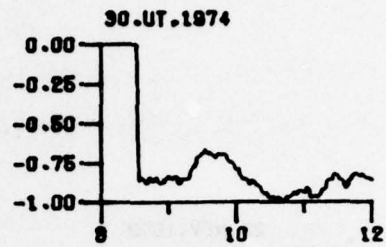
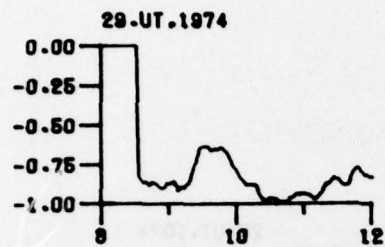


Figure C-4. (Contd)

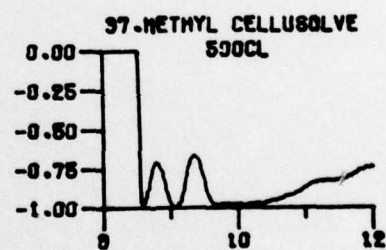
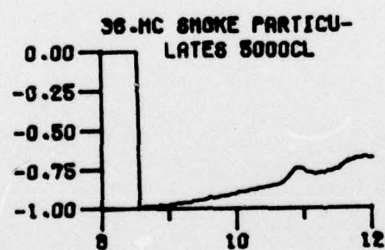
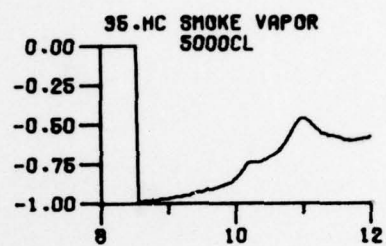
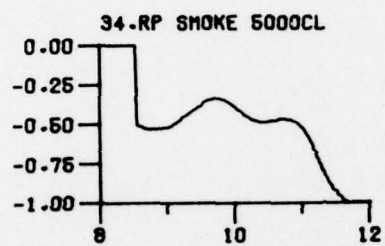


Figure C-5. LAB Simulated Contaminant Constraints

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